

NEWS	1	Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01 ChemPort single article sales feature unavailable
NEWS	3	JUN 01 CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS	4	JUN 26 NUTRACEUT and PHARMAML no longer updated
NEWS	5	JUN 29 IMSCOPROFILE now reloaded monthly
NEWS	6	JUN 29 EPFULL adds Simultaneous Left and Right Truncation (SLART) to AB, MCLM, and TI fields
NEWS	7	JUL 09 PATDPAFULL adds Simultaneous Left and Right Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS	8	JUL 14 USGENE enhances coverage of patent sequence location (PSL) data
NEWS	9	JUL 27 CA/Caplus enhanced with new citing references
NEWS	10	JUL 16 GBFULL adds patent backfile data to 1855
NEWS	11	JUL 21 USGENE adds bibliographic and sequence information
NEWS	12	JUL 28 EPFULL adds first-page images and applicant-cited references
NEWS	13	JUL 28 INPADOCDB and INPAFAMDB add Russian legal status data
NEWS	14	AUG 10 Time limit for inactive STN sessions doubles to 40 minutes
NEWS	15	AUG 18 COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	16	AUG 24 ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	17	AUG 24 CA/Caplus enhanced with legal status information for U.S. patents
NEWS	18	SEP 09 50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS	19	SEP 11 WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,  
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

**NEWS HOURS** STN Operating Hours Plus Help Desk Availability  
**NEWS LOGIN** Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 16:06:05 ON 23 SEP 2009

=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE ENTRY TOTAL SESSIONS  
FILL ESTIMATED COST 0.22 0.22

FILE 'REGISTRY' ENTERED AT 16:06:26 ON 23 SEP 2009  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with ZIC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 22 SEP 2009 HIGHEST RN 1186072-05-8  
DICTIONARY FILE UPDATES: 22 SEP 2009 HIGHEST RN 1186072-05-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

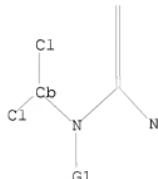
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10531783-broad.str

L1        STRUCTURE uploaded

=> d 11  
L1 HAS NO ANSWERS  
L1                    STR



G1 Me,Et,n-Pr,i-Pr

Structure attributes must be viewed using STN Express query preparation.

=> s 11  
SAMPLE SEARCH INITIATED 16:06:45 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 6241 TO ITERATE

32.0% PROCESSED        2000 ITERATIONS                          4 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:    ONLINE    \*\*COMPLETE\*\*  
                                  BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:      120083 TO    129557  
PROJECTED ANSWERS:            38 TO        460

L2        4 SEA SSS SAM L1

=> s 11 full  
FULL SEARCH INITIATED 16:06:49 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 126827 TO ITERATE

100.0% PROCESSED 126827 ITERATIONS  
SEARCH TIME: 00.00.03

248 ANSWERS

L3 248 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
186.36 186.58

FILE 'CAPLUS' ENTERED AT 16:07:33 ON 23 SEP 2009  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 23 Sep 2009 VOL 151 ISS 13  
FILE LAST UPDATED: 22 Sep 2009 (20090922/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/CAplus family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> s 13  
L4 127 L3

=> s 14 py not > 2003  
MISSING OPERATOR L4 PY  
The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 14 not py > 2003  
7813375 PY > 2003  
L5 82 L4 NOT PY > 2003

=> s 15 and ligand  
374492 LIGAND  
L6 0 L5 AND LIGAND

=> s 15 and affinity  
335097 AFFINITY  
L7 1 L5 AND AFFINITY

=> s 15 and support  
579048 SUPPORT  
L8 0 L5 AND SUPPORT

=> s 15 and solid  
1221171 SOLID  
L9 2 L5 AND SOLID

=> s 15 and Fab  
19564 FAB  
L10 0 L5 AND FAB

=> s 15 and IgG  
86381 IGG  
L11 0 L5 AND IGG

=> s 15 and human  
2261058 HUMAN  
L12 2 L5 AND HUMAN

=> s 15 and chromatography  
358201 CHROMATOGRAPHY  
L13 0 L5 AND CHROMATOGRAPHY

=> s 15 and column  
470328 COLUMN  
L14 0 L5 AND COLUMN

=> s 15 and matrix  
622387 MATRIX  
L15 0 L5 AND MATRIX

=> s 15 and immunology  
6097 IMMUNOLOGY  
L16 0 L5 AND IMMUNOLOGY

=> s 17 or 19 or l12  
L17 5 L7 OR L9 OR L12

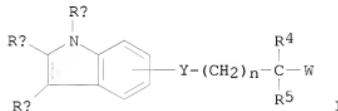
=> d l17 ibib abs hitstr 1-  
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

L17 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 2002:449646 CAPLUS  
DOCUMENT NUMBER: 137:33211  
TITLE: Preparation of N-indolylurea derivatives as peroxisome  
proliferator activated receptor  $\delta$  (PPAR  $\delta$ )  
activators  
INVENTOR(S): Takahashi, Toshihiro; Sakuma, Shogo; Endo, Tsuyoshi;  
Tendo, Atsushi; Yoshida, Shinichi; Kobayashi, Kunio;  
Mochiduki, Nobutaka; Yamakawa, Tomio; Kanda, Takashi;  
Masui, Seiichiro  
PATENT ASSIGNEE(S): Nippon Chemipharm Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 81 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002046154	A1	20020613	WO 2001-JP10576	20011204
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BE, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002024138	A	20020618	AU 2002-24138	20011204
PRIORITY APPLN. INFO.:			JP 2000-369890	A 20001205
			WO 2001-JP10576	W 20011204

OTHER SOURCE(S): MARPAT 137:33211  
GI



AB Urea derivs. represented by the general formula (I) or salts thereof [wherein Y = O, S; n = an integer of 0-4; R4, R5 = H, C1-8 alkyl optionally substituted by 1-3 of halogen atoms; W = CO2H, C2-8 alkoxy carbonyl, SO3H, cyano, tetrazolyl; a solid line accompanied by a dotted line represents a single or double bond; one of Ra, Rb, and Rc is R1N(R2)CON(R3)X and the other two groups are H, C1-8 alkyl, C6-10 aryl, C1-8 alkyl-C6-10 aryl; wherein R1, R2, R3 = H, C1-8 alkyl optionally substituted by 1-3 of halogen atoms, C1-8 alkoxy-C1-8 alkyl, C2-8 alkenyl, C2-8 alkynyl, C3-7 cycloalkyl, C3-7 cycloalkyl-C1-8 alkyl, C6-10 aryl, C6-10 aryl-C1-8 alkyl, heterocyclyl, heterocyclyl-C1-8 alkyl; X = C1-8 alkylene, remaining two R8 and R9 are each hydrogen or C1-8 alkyl; aryl, heterocyclyl, or aryl or heterocyclyl of arylalkyl or heterocyclylalkyl group is optionally substituted in Ra, Rb, and Rc] are prepared. These compds. are useful as blood sugar-lowering agents, hypolipidemics, antiobesity agents, hypcholesteremics, antiarteriosclerotics, anticancer agents, antiinflammatory agents, etc. Thus, 47 mg 2,4-dichlorophenyl isocyanate was added to a solution of 78 mg 2-[(1-[2-(isobutylamino)ethyl]indol-5-yloxy)-2-methylpropionic acid Et ester in EtOAc and stirred at room temperature for 0.5 h to give 83% 2-[(1-[2-(N'-2,4-dichlorophenyl-N-isobutylamino)ethyl]indol-5-yloxy)-2-methylpropionic acid Et ester which (96 mg) was dissolved in ethanol, treated with 1 M aqueous NaOH, stirred at room temperature for 16 h, treated with 0.1 M aqueous HCl under ice-cooling, and stirred at room temperature for 1 h to give 100% 2-[(1-[2-(N'-2,4-dichlorophenyl-N-isobutylureido)ethyl]indol-5-yloxy)-2-methylpropionic acid (II). In an assay for activating effect of PPAR $\delta$  receptor using CV-1 cells transfected with PPAR $\delta$  receptor-expressing plasmid, luciferase-expressing plasmid, and  $\beta$ -galactosidase-expressing plasmid, II at 10<sup>-5</sup> M exhibited 106% activation compared to L-165041.

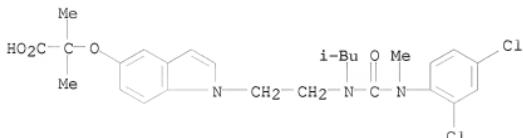
IT 435277-48-8P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of N-indolylurea derivs. as peroxisome proliferator activated receptor  $\delta$  (PPAR  $\delta$ ) activators for drugs)

RN 435277-48-8 CAPLUS

CN Propanoic acid, 2-[{[1-{[2-[(2,4-dichlorophenyl)methylamino]carbonyl}(2-methylpropyl)amino]ethyl}-1H-indol-5-yl]oxy}-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:175776 CAPLUS

DOCUMENT NUMBER: 137:279130

TITLE: Identification of a novel, orally bioavailable histamine H3 receptor antagonist based on the 4-benzyl-(1H-imidazol-4-yl) template

AUTHOR(S): Aslanian, Robert; Mutahi, Mwangi W.; Shih, Neng-Yang; McCormick, Kevin D.; Piwinski, John J.; Ting, Pauline C.; Albanese, Margaret M.; Berlin, Michael Y.; Zhu, Xiaohong; Wong, Shing-Chun; Rosenblum, Stuart B.; Jiang, Yueheng; West, Robert; She, Susan; Williams, Shirley M.; Bryant, Matthew; Hey, John A.

CORPORATE SOURCE: The Schering Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(6), 937-941

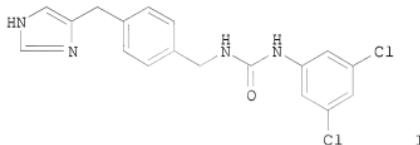
PUBLISHER: CODEN: BMCL8; ISSN: 0960-894X  
Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:279130

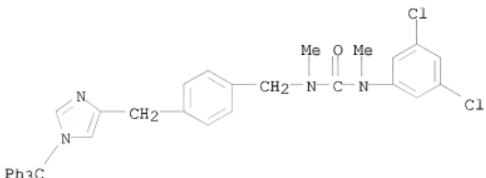
GI



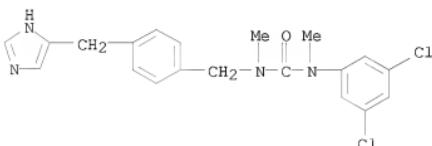
I

AB A novel series of histamine H3 receptor antagonists, based on the 4-benzyl-(1H-imidazole-4-yl) template, incorporating urea and carbamate linkers has been prepared. The urea I is a selective H3 antagonist and demonstrates excellent oral plasma levels in the rat and monkey.

IT 466671-37-4P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (preparation of imidazolylmethylbenzylureas as histamine H3 receptor  
 antagonists)  
 RN 466671-37-4 CAPLUS  
 CN Urea, N-(3,5-dichlorophenyl)-N,N'-dimethyl-N'-[{4-[(1-(triphenylmethyl)-1H-  
 imidazol-4-yl)methyl]phenyl}methyl]- (CA INDEX NAME)



IT 705264-28-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of imidazolylmethylbenzylureas as histamine H3 receptor  
 antagonists)  
 RN 705264-28-4 CAPLUS  
 CN Urea, N-(3,5-dichlorophenyl)-N'-[{4-(1H-imidazol-5-ylmethyl)phenyl}methyl]-  
 N,N'-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS  
 RECORD (24 CITINGS)  
 REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 2001:237842 CAPLUS  
 DOCUMENT NUMBER: 134:266205  
 TITLE: Preparation of collagen formation-inhibiting benzene  
 derivatives  
 INVENTOR(S): Kojima, Hiroshi; Sakamoto, Makoto; Yasumura, Koichi  
 PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 97 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001089412	A	20010403	JP 1999-269015	19990922

PRIORITY APPLN. INFO.:

JP 1999-269015

19990922

OTHER SOURCE(S):

MARPAT 134:266205

AB (R1)ac<sub>6</sub>H<sub>5</sub>-aBVWA [I; R1 = H, halo, OH, NO<sub>2</sub>, cyano, etc.; a = 1-5; V = NHCO, CONH, NHCONH, NHC(S)NH, SCH<sub>2</sub>CONH, etc.; B = p-C<sub>6</sub>H<sub>4</sub>, (un)substituted pyridine-2,5-diyl, pyrimidine-2,5-diyl, pyrazine-2,5-diyl, pyridine-2,3-diyl; W = O, S, SO, NH, CO, CH<sub>2</sub>, SO<sub>2</sub>; A = aryl] or their salts, useful for treatment of lung or liver fibrosis, are prepared 3,4,5-Trimethoxybenzoic acid (440 mg) was amidated by 500 mg 3-amino-6-(4-tert-butylphenoxy)pyridine in the presence of 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide.HCl and 1-hydroxybenzotriazole in DMF at room temperature for 1 day to give 750 mg I [(R1)a = 3,4,5-(OMe)<sub>3</sub>, V = CONH, B = pyridine-2,5-diyl, W = O, A = C<sub>6</sub>H<sub>4</sub>CMe<sub>3</sub>-p]. I [(R1)a = 3,4-C<sub>12</sub>, V = CONH, B = p-C<sub>6</sub>H<sub>4</sub>, W = O, A = 5-oxo-5,6,7,8-tetrahydronaphthalen-1-yl] in vitro inhibited TGF $\beta$ -1-induced collagen synthesis in human LI90 cells with IC<sub>50</sub> of 2.37  $\mu$ M.

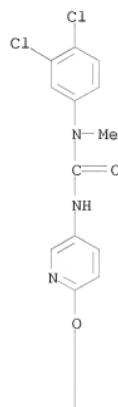
IT 332009-21-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of collagen formation-inhibiting benzene derivs.)

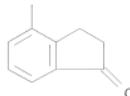
RN 332009-21-9 CAPLUS

CN Urea, N-(3,4-dichlorophenyl)-N'-(6-[(2,3-dihydro-1-oxo-1H-inden-4-yl)oxy]-3-pyridinyl)-N-methyl- (CA INDEX NAME)

PAGE 1-A

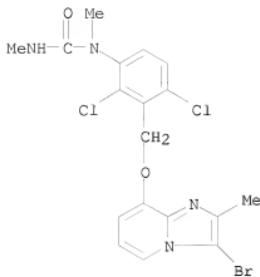


PAGE 2-A



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

L17 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 1998:66714 CAPLUS  
DOCUMENT NUMBER: 128:136098  
ORIGINAL REFERENCE NO.: 128:26594h,26595a  
TITLE: A Novel Class of Orally Active Non-Peptide Bradykinin B2 Receptor Antagonists. 1. Construction of the Basic Framework  
AUTHOR(S): Abe, Yoshito; Kayakiri, Hiroshi; Satoh, Shigeki; Inoue, Takayuki; Sawada, Yuki; Imai, Keisuke; Inamura, Noriaki; Asano, Masayuki; Hatori, Chie; Katayama, Akira; Oku, Teruo; Tanaka, Hirokazu  
CORPORATE SOURCE: Exploratory Research Laboratories, Fujisawa Pharmaceutical Co., Ibaraki, 300-26, Japan  
SOURCE: Journal of Medicinal Chemistry (1998), 41(4), 564-578  
PUBLISHER: CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: American Chemical Society  
LANGUAGE: English  
AB A novel class of potent, selective, and orally active non-peptide bradykinin (BK) B2 receptor antagonists were designed and synthesized starting from 8-benzoyloxyimidazo[1,2- $\alpha$ ]pyridine derivative(I). The unique screening lead I was discovered by a 2-step intentional random screening process, involving recognition of the relationship between BK and angiotensin II (Ang II) and the common structural features. Systematic chemical modification of I elucidated the structural requirements essential for B2 binding affinity leading to the identification of 8-[(3-(N-acylglycyl-N-methylamino)-2,6-dichlorobenzyl)oxy]-3-halo-2-methyylimidazo[1,2- $\alpha$ ]pyridine skeleton as the basic framework of this new series of B2 antagonists. A mol. modeling study suggested the key role of the N-methylanilide moiety at the 3-position of the 2,6-dichlorobenzene ring to allow these compds. to adopt the characteristic active conformation. The representative lead compds. inhibited the specific binding of [<sup>3</sup>H]BK to guinea pig ileum membrane preps. expressing B2 receptors, with nanomolar IC<sub>50</sub>s and also displayed in vivo functional antagonistic activities against BK-induced bronchoconstriction in guinea pigs at an oral dose of 1 mg/kg. Pharmacokinetic studies of the N-butylamide and Et urea moieties at the 3-position of the 2,6-dichlorobenzene in rats highlighted their excellent oral bioavailabilities, indicating that they represent the first orally active non-peptide B2 antagonists reported to date.  
IT 160642-24-0P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and MSBAR of nonpeptide bradykinin B2 receptor antagonists)  
RN 160642-24-0 CAPLUS  
CN Urea, N-[3-[(3-bromo-2-methyylimidazo[1,2- $\alpha$ ]pyridin-8-yl)oxy]methyl]-2,4-dichlorophenyl-N,N'-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 69 THERE ARE 69 CAPLUS RECORDS THAT CITE THIS RECORD (70 CITINGS)  
 REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 1967:508325 CAPLUS  
 DOCUMENT NUMBER: 67:108325  
 ORIGINAL REFERENCE NO.: 67:20403a,20406a  
 TITLE: Tuberculosstatic urea derivatives  
 INVENTOR(S): Gagneux, Andre R.; Frick, Wilhelm  
 PATENT ASSIGNEE(S): Geigy, J. R., A.-G.  
 SOURCE: Ger., 5 pp.  
 CODEN: GWXXAW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1246722	-----	19670810	DE 1966-G48486	19661117
CH 456570	-----		CH	
FR 1504098	-----		FR	
FR 6433	-----		FR	
GB 1125559	-----		GB	
US 3539626	-----	19701110	US	19681212
US 3621040	-----	19710000	US	
US 3621100	-----	19711116	US	19681118
PRIORITY APPLN. INFO.:	-----		CH	19651118

AB The title compds. are prepared by treating a) adamantlylamines with an aryl isocyanate, aryl isothiocyanate, or a carbanilic or thiocarbanilic acid derivative; b) an adamantly isocyanate, isothiocyanate, carbamate, or thiocarbamate with an aryl amine; or c) an adamantly and aryl substituted carbodiimide with H2O or H2S. Thus, a mixture of 36.5 millimoles 1-adamantylamine in 100 ml. absolute C6H6 and 33.3 millimoles 3,4-dichlorophenyl isocyanate in 100 ml. absolute C6H6 is heated at 80° 1 hr. and cooled and the filtered solid stirred 1 hr. in 100 ml. N HCl to give 1-(1-adamantyl)-3-(3,4-dichlorophenyl)urea, m. 220-1°. Similarly prepared are the following substituted 1-(1-adamantyl)ureas (substituents and m.p. given): 3-(p-MeC6H4), 252-6°; 3-(p-C1C6H4), 242-3°; 3-(2,4-C12C6H3), 221-2°; 3-[6,3-C1(F3C)C6H3], 233-4°; 3-(o-MeOC6H4), 234-6°; 3-(p-MeOC6H4), 235-8°; 3-[2,5(MeO)2C6H3], 240-2°; 3-(m-AccC6H4), 200-4°; 1-Me-3-(3,4-C12C6H3), 193-5°; 3-Me-3-(3,4-C12C6H3), 180-2°. Also prepared are

1-(1-adamantyl)thioureas: 3-(p-C<sub>1</sub>C<sub>6</sub>H<sub>4</sub>), 172-3°; 3-(2,4-C<sub>12</sub>C<sub>6</sub>H<sub>3</sub>), 181-3°; 3-[4,3-C<sub>1</sub>(F<sub>3</sub>C)C<sub>6</sub>H<sub>3</sub>], 169-71°; and 3-(3,4-C<sub>12</sub>C<sub>6</sub>H<sub>3</sub>) (I), 189-92°. Similarly prepared are  
 1-(1-adamantylmethyl)-3-(3,4-dichlorophenyl)urea, m. 189-91°;  
 1-( $\alpha$ -methyl-1-adamantylmethyl)-3-(3,4-dichlorophenyl)urea, m. 195-8°; 1-(tricyclo[4.3.1.13,8]undec-3-yl)-3-(3,4-dichlorophenyl)urea, m. 233-6°; and  
 1-(2-oxaadamant-1-yl)-3-(3,4-dichlorophenyl)urea, m. 208-10°. To a mixture of 15 millimoles I in 600 ml. absolute dioxane is added 50 millimoles anhydrous MgSO<sub>4</sub> and 120 millimoles PbO, the mixture stirred at 60° 15 hrs., cooled, and filtered, the filtrate taken to dryness in vacuo, the oily residue dissolved in 300 ml. pentane, the turbid solution filtered through C, and the filtrate concentrated to give  
 1-(1-adamantyl)-3-(3,4-dichlorophenyl)carbodiimide, m. 60-1° (pentane). A mixture of 50 millimoles bicyclo[3.3.1]nonane-3,7-dione and 50 millimoles PhCH<sub>2</sub>NH<sub>2</sub> in 300 ml. tetrahydrofuran is refluxed 0.5 hr., cooled, and added with stirring to 100 millimoles LiAlH<sub>4</sub> in 100 ml. absolute Et<sub>2</sub>O, the mixture stirred at 40° 6 hrs., 19 ml. N NaOH added with ice-cooling, the precipitate filtered off, the filtrate evaporated, the residue dissolved in 500 ml. Me<sub>2</sub>CO, and 5 ml. concentrated HCl added, to afford N-benzyl-2-oxaadamantylamine - HCl (II), m. 242-5°. A solution of 33 millimoles II in 100 ml. EtOH is hydrogenated with 50 atmospheric H in the presence of 2 g. 5% Pd-C at 100° 2 hrs., the mixture cooled and filtered, the filtrate evaporated, 25 ml. concentrated NaOH solution added to the residue, the mixture extracted with Et<sub>2</sub>O, the Et<sub>2</sub>O evaporated, and the residue sublimed at 60° and 0.1 mm. to yield 2-oxaadamantylamine, m. 148-54°; hydrochloride m. 280°.  
**IT**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
**RN** 16192-94-2 CAPLUS  
**CN** Urea, N-(3,4-dichlorophenyl)-N-methyl-N'-tricyclo[3.3.1.13,7]dec-1-yl-  
 (CA INDEX NAME)

